

Status of SG38

Presented to CSEWG: Brookhaven National Laboratory

8 May 2015

Bret Beck



LLNL-PRES-??????

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC



Outline

- How new structure effort got started
- OECD/NEA WPEC subgroup 38
 - 7 tasks (project creep)
 - Status
- FUDGE and GND

How new structure effort got started

History of evaluated formats – LLNL's ENDL

- Evaluated Nuclear Data Library
- AWE designed a format in the late 1950s
- Shared it with LLNL
 - LLNL modified it some
 - Have used it since ~1960 (~54 years old)
- Format
 - Only supports pointwise data
 - All data in lab. frame except 2-body $P(\mu|E)$
- Only LLNL uses it
 - This has effectively isolated us from the rest of the community

LLNL needed a new format

- Around 2006 we (LLNL) started search for new format.
- Decided against ENDF
- Started design of GND
 - GND = Generalize Nuclear Data
- Took design to CSEWG ~ Nov 2011
 - Recommended we make a WPEC proposal
- Dennis McNabb made proposal to WPEC May 2012

Original proposal to WPEC by McNabb

LLNL has made an initial attempt at a new format, which can be downloaded at <https://ndclx4.bnl.gov/gf/project/gnd/>

- Sub-group participants will
 - Develop a common data model for reaction data
 - Agree on best practices and how to “enforce” them
 - Test things out with their local ENDF-formatted databases
 - Propose a process for dissemination and future modifications
- LLNL and USNDP is committed to seeing this through
- Benefits are significant
 - Attract and retain next generation of scientists and engineers
 - Leverage significant infrastructure that will continue to evolve
 - Overcomes limitations of existing format in an extensible way
 - Positions community to link disparate data products to each other

SG38 formed

- Title

**“Beyond the ENDF format:
A modern nuclear database structure”**

- OECD/NEA WPEC subgroup 38
- Started as a task to design a new nuclear data structure to replace ENDF6.
 - Project creep?

Schedule

- Meet every 6 months for 3 years.
- First meeting Nov. 2012.
- Tried video conferencing. This is not working in my opinion.
- Since last meeting in Dec 2014, USA has had 3 sub-meetings (sub-verse?).
 - Caleb and me to LANL. LANL to LLNL. LLNL, LANL, BNL to ORNL.
 - Need to have more of these, in my opinion. Everybody welcome.
- Next WPEC meeting this May. Last meeting Nov 2015. Will ask for one year extension.

New nuclear data structure vs. format

- SG 38 is defining a new structure for nuclear 'reaction' data
 - This is an outline of how the data are to be stored
- SG 38 has agreed to support an XML version of GND
 - We call XML a meta-language
- A format is a structure represented using a meta-language
 - E.g., GND/XML, GND/HDF5, GND/Python

7 SG 38 tasks – decided at first meeting – project creep?

- Low-level data containers
 - Similar to ENDF LIST, TAB1, TAB2, etc.
 - Work with other data projects (e.g., ENSDF, EXFOR, RIPL)
- Hierarchy for storing particle data and nuclear level schemes and decay data
- Top-level hierarchy for storing nuclear reaction data
- Infrastructure for data handling, processing, plotting, etc.
- API for reading and writing data in the new structure
- Defining the tests that will be needed to assure quality of data
- Documentation and governance

Outline for each task

- Develop a requirements document
- Develop a specifications document

Low-level data containers

- Low-level data containers
 - Draft requirements and specifications document written.
 - 61 pages
- Hierarchy for storing particle data and nuclear level schemes and decay data
- Top-level hierarchy for storing nuclear reaction data
- Infrastructure for data handling, processing, plotting, etc.
- API for reading and writing data in the new structure
- Defining the tests that will be needed to assure quality of data
- Documentation and governance

Low-level data containers

- Low-level data containers
- Hierarchy for storing particle data and nuclear level schemes and decay data
 - Draft requirements and specifications document written.
 - 29 pages
- Top-level hierarchy for storing nuclear reaction data
- Infrastructure for data handling, processing, plotting, etc.
- API for reading and writing data in the new structure
- Defining the tests that will be needed to assure quality of data
- Documentation and governance

Low-level data containers

- Low-level data containers
- Hierarchy for storing particle data and nuclear level schemes and decay data
- Top-level hierarchy for storing nuclear reaction data
 - Draft requirements document written.
 - ~91 pages – thank you Dave.
- Infrastructure for data handling, processing, plotting, etc.
- API for reading and writing data in the new structure
- Defining the tests that will be needed to assure quality of data
- Documentation and governance

FUDGE and GND

LLNL's infrastructure - FUDGE

- For Updating Data and Generating ENDL
- Started around 2002 to supporting managing and processing LLNL's ENDL data
- Interface written in Python
 - Has C/C++ routines for computationally intensive calculations
- Modified to support the new format (GND)
 - More modification needed as GND changes

FUDGE

- Read/write ENDL, ENDF6 and GND/XML
 - Translation between ENDF6 and GND/XML
- Modifying data
 - e.g., $xSecMod = 1.2 * xSec$
- Viewing data: plotting and printing
- Checking
 - Finds issues other checkers miss
 - used in BNL/NNDC's ADVANCE package
- Processing

Status of FUDGE ENDF translation to GND

- For ENDF-VII.1 sub-libraries:
 - Can translate:
 - neutrons/ protons/ deuterons/ tritons/ helium3s gammas/ standards/ electrons/ photoat/ atomic_relax/
 - Can be translated into GND-like format, these are not yet integrated with Fudge:
 - nfy/ sfy/ thermal_scatt/
 - Currently not supported:
 - Decay/
- Newest FUDGE
 - One day needed to implement a few missing features in latest “specifications”.
 - Should also handle other libraries (e.g., JEFF, JENDL) as long as the data are good.

Summary

- Low-level data containers
 - Requirements and specifications document written
- Hierarchy for storing particle data and nuclear level schemes and decay data
 - Requirements and specifications document written
- Top-level hierarchy for storing nuclear reaction data
 - Requirements document written
- Infrastructure for data handling, processing, plotting, etc.
- API for reading and writing data in the new structure
- Defining the tests that will be needed to assure quality of data
- Documentation and governance

Glad to give current documents to anyone.

Summary – cont.

- LLNL will have a working version of “GND” by Oct 1 2015.
 - We need something as ENDL is too limiting.
- FUDGE is nearly up to date with latest ‘design’.
 - Will be up to date by Oct 1 2015.
 - Additional questions to beck6@llnl.gov or mattoon1@llnl.gov

FUDGE is freely available and can be downloaded at
<https://ndclx4.bnl.gov/gf/project/gnd/>

History of evaluated formats - ENDF

- Evaluated Nuclear Data File
- Designed in the early 1960s (~50 years old)
- Supports pointwise and parametric data type
- Data can be in lab or center-of-mass
- Obviously richer than ENDL but still has issues
 - Limits values to 11 character each
 - e.g., “-1.2345e-10”. Often written without “e” (e.g., “-1.23456-10”) to get another digit which requires special handling for all computer languages but FORTRAN
 - Punchcard form
 - Fixed particle and reaction types